

09601762

Welcome to STN International! Enter x:x

LOGINID:sssptal202sxq

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded  
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded  
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS  
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 28 Oct 21 EVENTLINE has been reloaded  
NEWS 29 Oct 24 BEILSTEIN adds new search fields  
NEWS 30 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 31 Oct 25 MEDLINE SDI run of October 8, 2002  
NEWS 32 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 33 Nov 25 More calculated properties added to REGISTRY  
  
NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

12/1/02

09601762

specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 17:15:59 ON 01 DEC 2002

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:16:05 ON 01 DEC 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

DICTIONARY FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNnote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s 4-bromo-2-methoxyestradiol

11862466 4

938248 BROMO

14553906 2

22 METHOXYESTRADIOL

L1

1 4-BROMO-2-METHOXYESTRADIOL

(4 (W) BROMO (W) 2 (W) METHOXYESTRADIOL)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.38	16.59

FILE 'CAPLUS' ENTERED AT 17:16:38 ON 01 DEC 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

12/1/02

09601762

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 1 Dec 2002 VOL 137 ISS 23  
FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d ll ibib hitstr abs  
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN  
SAM - Index Name, MF, and structure - no RN  
FIDE - All substance data, except sequence data  
IDE - FIDE, but only 50 names  
SQIDE - IDE, plus sequence data  
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used  
SQD - Protein sequence data, includes RN  
SQD3 - Same as SQD, but 3-letter amino acid codes are used  
SQN - Protein sequence name information, includes RN  
  
CALC - Table of calculated properties  
EPROP - Table of experimental properties  
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

12/1/02

09601762

APPS -- Application and Priority Information  
BIB -- CA Accession Number, plus Bibliographic Data  
CAN -- CA Accession Number  
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels  
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):end

=> d 11 ibib hitstr abs  
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:N

=> s 11  
L2 2 L1

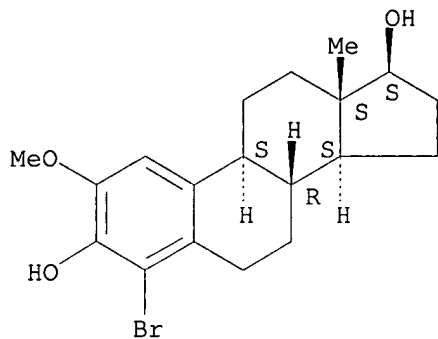
=> d 12 1-2 ibib hitstr abs

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1989:633338 CAPLUS  
DOCUMENT NUMBER: 111:233338  
TITLE: Preparations of 2,4-disubstituted estradiols  
AUTHOR(S): Pert, Derek J.; Ridley, Damon D.  
CORPORATE SOURCE: Dep. Org. Chem., Univ. Sydney, Sydney, 2006, Australia  
SOURCE: Australian Journal of Chemistry (1989), 42(3), 421-32  
CODEN: AJCHAS; ISSN: 0004-9425  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 111:233338  
IT 97515-50-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
RN 97515-50-9 CAPLUS  
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)  
(CA INDEX NAME)

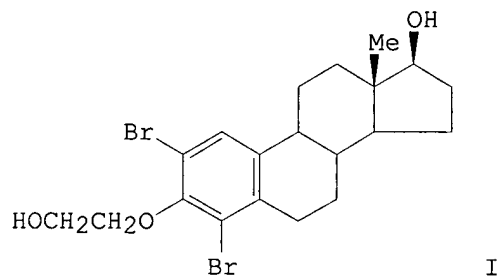
12/1/02

09601762

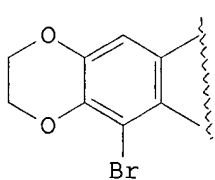
Absolute stereochemistry.



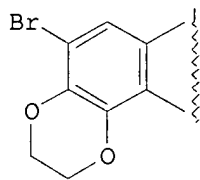
GI



I



II



III

AB Dibromoestradiol I was treated with  $\text{CuCl}_2/\text{NaOMe}$  to give [2,3]dioxane II as the major product as well as a minor amt. of the [3,4]dioxane deriv. III. The compds. were used to prep. a no. of 2,4-disubstituted estradiol derivs. Alternative routes to other 2,4-disubstituted estradiols are described.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:465176 CAPLUS

DOCUMENT NUMBER: 103:65176

TITLE: Catechol formation of fluoro- and bromo-substituted estradiols by hamster liver microsomes. Evidence for dehalogenation

AUTHOR(S): Li, Jonathan J.; Purdy, Robert H.; Appelman, Evan H.; Klicka, John K.; Li, Sara Antonia

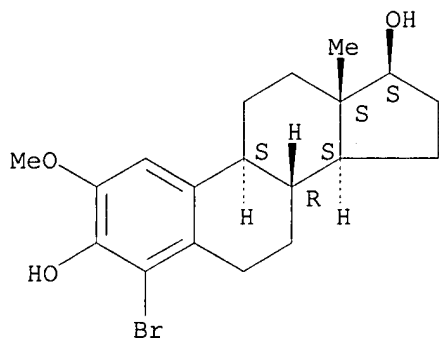
CORPORATE SOURCE: Med. Res. Lab., Veterans Adm. Med. Cent., Minneapolis, MN, 55417, USA

12/1/02

09601762

SOURCE: Molecular Pharmacology (1985), 27(5), 559-65  
CODEN: MOPMA3; ISSN: 0026-895X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 97515-50-9  
RL: FORM (Formation, nonpreparative)  
(formation of, from halogenated estrogens by liver microsome)  
RN 97515-50-9 CAPLUS  
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



AB Liver microsomes from castrated hamsters were incubated with 2-fluoro-, 4-fluoro-, or 2,4-difluoroestradiols and analogous bromo-substituted estradiols to det. the extent of 2- and 4-hydroxylation with these substrates. Estrogen 2-hydroxylase [9055-96-3] and estrogen 4-hydroxylase [80237-93-0] activity was detd. by radioenzymic assay, and the 3H-labeled monomethyl ether products were identified by HPLC. With unsubstituted 17.beta.-estradiol [50-28-2] as substrate, 97% of the product formed was 2-hydroxylated, and 3% was 4-hydroxylated. The monosubstituted fluoroestradiols exhibited >2-fold enhanced ability to form catechol estrogens compared with their corresponding bromoestradiols. Data presented indicated substantial defluorination when 2-fluoroestradiol [16205-32-6] was the substrate, which amounted to 36% of the total product formed, and 32% of the rate of 2-hydroxylation found with unsubstituted 17.beta.-estradiol as substrate. Interestingly, the rate of 4-hydroxylation was elevated 20- and 6.7-fold, resp., when 2-fluoroestradiol and 2,4-difluoroestradiol [97515-43-0] were the substrates compared to the rate with 17.beta.-estradiol. Moreover, both 4-fluoroestradiol [1881-37-4] and 2,4-difluoroestradiol exhibited at least a 1.6-fold greater rate of 2-hydroxylation compared with 17.beta.-estradiol. In contrast, the rate of dehalogenation with 2-bromoestradiol [15833-07-5] was only 12% of that found with 2-fluoroestradiol. No debromination was obtained with 4-bromoestradiol [1630-83-7] and essentially no catechols were formed using 2,4-dibromoestradiol [19590-55-7] as substrate with these hamster liver microsomes. These data provide evidence for defluorination of these substituted estrogens, particularly at the C-2 position, and seriously hamper the use of fluoroestrogens in studies of hormonal carcinogenicity.